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Excitation of hydrogen atom in the high energy region

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Abstract : The first-Born approximation is used to evaluate the cross section for excitation of hydrogen atom by proton and other bare nuclei (He^{2+}, Li^{9+}, C^{6+}, O^{8+}, Si^{14+}, Fe^{26+}) etc. from any arbitrary state (nlm) to any other arbitrary excited state (n′l′m′) for incident energies in the range of 100 Kev to 10 Mev. A comparative study is made by taking values from the empirical formula by Lodge *et al* [1].

Keywords : Excitation cross sections, hydrogen atom, first-Born approximation

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Ion-atom collision processes directly relevant to supplementary heating energy loss and particle distribution in magnetically confined fusion plasmas are being studied theoretically. The presence of small fractions of impurity ions of hydrogen, helium, carbon, oxygen, silicon and iron or any other element inside the container of plasma creates problems for smooth neutral hydrogen beam penetration into fusion plasma. The excitations of penetrating atomic hydrogen beam by collisions with impurity ions leads to serious power loss and is a competitive process with charge transfer and ionization. Most of the calculated results reported so far are on the excitation of ground state atomic hydrogen by heavy ions [2-7]. To have an extensive data set from the arbitrary initial excited states to arbitrary final excited states of atomic hydrogen by ion impact, we have calculated the following processes :

$A^{Q+} + H(n,l,m) \rightarrow A^{Q+} + H(n',l',m')$ in the frame work of first Born approximation (FBA) upto a fairly large value of excitations. Mondal *et al* [8] have calculated total cross sections for H(1s) excitations upto n′=20. In this paper, we have calculated cross sections from different initial excited states.

The transition amplitude from any arbitrary state (nlm) to any arbitrary state (n′l′m′) in the framework of FBA is.

$$T_{if}^{FBA} \equiv \langle \psi_f | V_i | \psi_i \rangle \tag{1}$$

where,

$$\psi_i = \phi_{nlm}(r_T) e^{i k_i \cdot R_T} \quad ; \quad \psi_f = \phi_{n'l'm'}(r_T) e^{i k_f \cdot R_T}$$

with $\phi_{nlm}(r_T)$ and $\phi_{n'l'm'}(r_T)$ are hydrogenic wave functions. The eq. (1) may be written as

$$T_{if}^{FBA} = -2\mu_i Z_p a^2 \int dr_T \phi^*_{n'l'm'}(r_T)\phi_{nlm}(r_T)e^{iq'\cdot r_T} \tag{2}$$

where $\mu_i = M_p(1+M_T)/(1+M_p+M_T)$, $a = M_T/(1+M_T)$, M_p and M_T being the projectile and target mass respectively. Z_p is the charge of projectile, $q' = a(k_i - k_f)$, k_i, k_f being the initial and final momentum vector and $r_T = 1/a(r_p + R_T)$ (see Figure 1). (Atomic units are used unless otherwise stated). The final expression for the transition amplitudes are

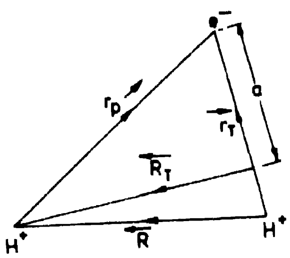

Figure 1. Coordinates for (H^+–H) system.

$$T_{if}^{FBA} = -4\pi\mu_i Z_p a^2(-1)^{m'} \sum_{L=0}^{\infty}\sum_{M=-L}^{L}\sum_{K=0}^{n-l-1}\sum_{K'=0}^{n'-l'-1} C_N C_{N'} Y^*_{LM}(\hat{q}') .$$

$$(q')^{L-2}(i)^L \frac{1}{2^{L+1}}\frac{1}{\beta^{L+M1+3}}\frac{\Gamma(L+M1+3)}{\Gamma(L+3/2)} .$$

$${}_2F_1\left(\frac{L+M1+3}{2},\frac{L+M1+4}{2}, L+3/2;-q'^2/\beta'^2\right).$$

$$\{(2L+1)(2l+1)(2l'+1)\}^{1/2} .$$

$$C(L,l,l',0,0,0)C(L,l',l,M,-m',m), \tag{3}$$

C_N, $C_{N'}$ are normalization constant of the initial and final wave function of hydrogen atom. $M_1 = l+l'+k+k'$ and $\beta = \lambda+\lambda'$, λ and λ' being the screening *c* constants, C's are the Clebsch-Gordan coefficients.

Computed results obtained for H^+–H collision case is presented in the Table 1 for projectile energies varying from 100 keV to 10 Mev for initial states n=2 to n=5. We have computed excitation cross sections upto the final state with n′=15. We have however presented in the Table 1, results for a few selected excited states and have not shown explicitly results for each indi‹idual subshell *l*. The sum of the cross sections obtained from different *l* values only are presented here. Detailed results may be supplied on request.

At high energies of 100 keV/amu and above, the computed results in the FBA are fairly reliable. One of the advantages of the FBA calculation is that, one can easily calculate the excitation cross section results by the impact of fully stripped ions of He^{2+}, C^{6+}, O^{8+},

Si^{14+}, Fe^{26+} etc, if one takes velocity as the parameter for the cross sections and the corresponding incident projectile energy is obtained accordingly. The relevant cross sections for various projectile ions can be obtained by suitably changing the Z_p values according to eq. (3).

Table 1. Cross sections (σn) in units of 10^{-16} cm^2. Numbers in brackets represent the power of 10 by which each entry should be multiplied.

Energy (keV/amu)	Initial state	σ_3	σ_4	σ_5	σ_6	σ_7	σ_8	σ_9	σ_{10}
100	2	3.617 (1)	6.923	2.615	1.301	0.747	0.475	0.320	0.227
500	2	8.001	1.564	0.574	0.292	0.169	0.108	0.073	0.052
1000	2	4.053	0.786	0.302	0.149	0.087	0.054	0.036	0.024
5000	2	0.818	0.159	0.059	0.029	0.012	0.010	0.006	0.004
10000	2	0.408	0.078	0.029	0.014	0.009	0.042 (-1)	0.037 (-1)	0.002
100	3		1.281 (2)	5.042 (1)	1.900 (1)	9.622	5.482	3.505	2.399
500	3		5.265 (1)	1.051 (1)	3.985	1.995	1.156	0.739	0.608
1000	3		2.643 (1)	5.277	2.038	1.004	0.579	0.367	0.250
5000	3		5.298	1.051	0.399	0.216	0.116	0.079	0.058
10000	3		2.647	0.525	0.198	0.099	0.057	0.035	0.025
1000	5				2.612 (2)	5.409 (1)	2.078 (1)	1.007 (1)	5.844
5000	5				5.335 (1)	1.083 (1)	4.309	2.074	1.187

There exist formidable difficulties in finding a unified theory of excitation, which would be valid for the entire region and all quantum numbers. Lodge *et al* [1] obtained a formula on the basis of quantal, semiclassical and classical methods. The excitations from ground state to excited states n′ (n′<10) agree very well, but for higher initial state (n>1), differences between calculated cross sections and values obtained from [1] increase with the increase of n. This differences also increase with the increase of excited states for a fixed initial state and energy.

Acknowledgments

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